

Integrative Structure Validation Report ?

February 18, 2025 - 08:34 AM PST

The following software was used in the production of this report:

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

PDB ID	9A2A
PDB-Dev ID	PDBDEV_00000152
Structure Title	Integrative structure of the human MHM complex
Structure Authors	Arvindekar S; Jackman MJ; Low JKK; Landsberg MJ; Mackay JP; Viswanath S
Deposited on	2022-07-30

This is a PDB-IHM IM Structure Validation Report for a publicly released PDB-IHM entry.

We welcome your comments at helpdesk@pdb-ihm.org

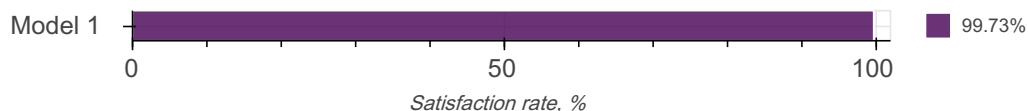
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

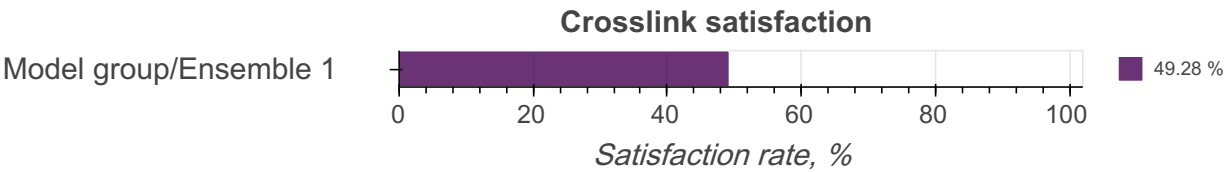
List of references used to build this report is available [here](#).

Overall quality ?

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: Excluded Volume Analysis





Ensemble information ?

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 1 model(s). A total of 17 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1	1	MTA1	A	431	1-164, 165-333, 334-353, 389-431	229-236, 354-388	100.00 / 91.88	Multiscale: Coarse-grained: 1 - 30 residue(s) per bead
				B					
		2	HDAC1	C	482	8-376	1-7, 377-482	100.00 / 76.56	Multiscale: Coarse-grained: 1 - 30 residue(s) per bead
				D					
		3	MBD3	E	291	1-71, 221-249	72-220, 250-291	100.00 / 34.36	Multiscale: Coarse-grained: 1 - 30 residue(s) per bead
				F					
		4	P66A	G	633	137-178	136	6.79 / 97.67	Coarse-grained: 1 residue(s) per bead
				H					

Datasets used for modeling ?

There are 17 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
14	Crosslinking-MS data	Zenodo	10.5281/zenodo.6674232
15	Crosslinking-MS data	Zenodo	10.5281/zenodo.6674232
2	Comparative model	Zenodo	10.5281/zenodo.6674232
4	De Novo model	Zenodo	10.5281/zenodo.6674232
6	Comparative model	Zenodo	10.5281/zenodo.6674232
7	Comparative model	Zenodo	10.5281/zenodo.6674232
8	De Novo model	Zenodo	10.5281/zenodo.6674232
9	Comparative model	Zenodo	10.5281/zenodo.6674232
12	Experimental model	Zenodo	10.5281/zenodo.6674232
13	Experimental model	Zenodo	10.5281/zenodo.6674232
17	3DEM volume	Zenodo	10.5281/zenodo.6674232
1	Experimental model	PDB	2FVU
3	Experimental model	PDB	4BKX
10	Experimental model	PDB	6CC8
5	Experimental model	PDB	2GAT
11	Experimental model	PDB	2L2L
16	3DEM volume	EMDB	EMD-21382

Methodology and software ?

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Sampling	Replica exchange monte carlo	None	600000	False	True

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	2.16.0	integrative model building	https://integrativemodeling.org
2	Integrative Modeling Platform (IMP)	2.16.0	integrative model building	https://integrativemodeling.org

Data quality ?

Crosslinking-MS

At the moment, data validation is only available for crosslinking-MS data deposited as a fully [compliant](#) dataset in the [PRIDE Crosslinking](#) database. Correspondence between crosslinking-MS and entry entities is established using [pyHMMER](#). Only residue pairs that passed the reported threshold are used for the analysis. The values in the report have to be interpreted in the context of the experiment (i.e. only a minor fraction of in-situ or in-vivo dataset can be used for modeling).

Crosslinking-MS dataset is not available in the [PRIDE Crosslinking](#) database.

3DEM volume

Validation for this section is under development.

Model quality ?

For models with atomic structures, MolProbity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Excluded volume satisfaction ?

Excluded volume satisfaction for the models in the entry are listed below. The Analysed column shows the number of particle-particle or particle-atom pairs for which excluded volume was analysed.

Model ID	Analysed	Number of violations	Excluded Volume Satisfaction (%)
1	1677196	4505	99.73

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

Restraint types are summarized in the table below. Restraints assigned "[by-residue](#)" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "[coarse-grained](#)". [Restraint group](#) represents a set of crosslinking restraints applied collectively in the modeling.

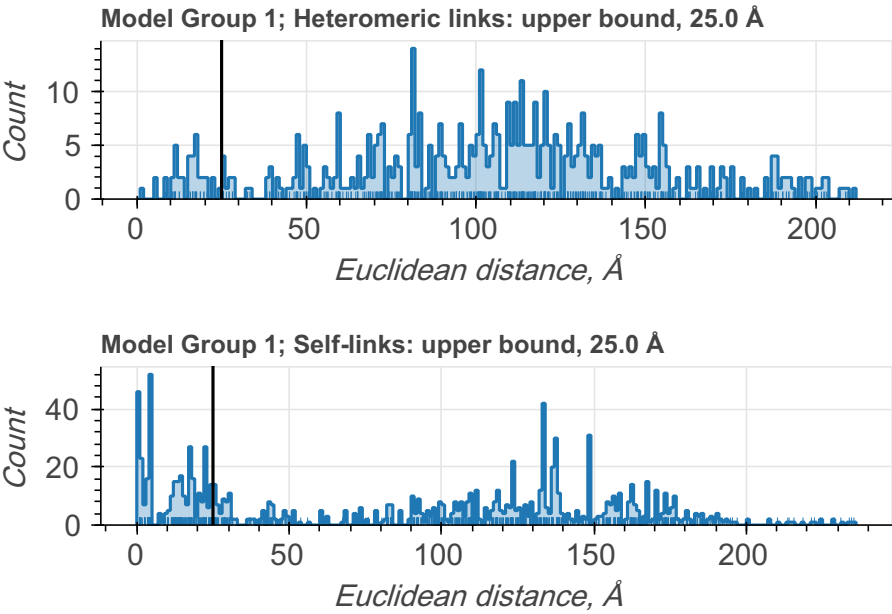
There are 1672 crosslinking restraints combined in 418 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BS3	LYS	CA	SER	CA	upper bound	25.0	220
BS3	LYS	coarse-grained	SER	coarse-grained	upper bound	25.0	364
BS3	SER	coarse-grained	SER	coarse-grained	upper bound	25.0	80
BS3	SER	CA	TYR	CA	upper bound	25.0	20
BS3	LYS	coarse-grained	LYS	coarse-grained	upper bound	25.0	356

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BS3	LYS	coarse-grained	THR	coarse-grained	upper bound	25.0	92
BS3	ARG	CA	SER	CA	upper bound	25.0	24
BS3	LYS	CA	LYS	CA	upper bound	25.0	128
BS3	SER	coarse-grained	TYR	coarse-grained	upper bound	25.0	8
BS3	ARG	CA	ARG	CA	upper bound	25.0	8
BS3	SER	CA	SER	CA	upper bound	25.0	60
BS3	LYS	CA	TYR	CA	upper bound	25.0	68
BS3	SER	coarse-grained	THR	coarse-grained	upper bound	25.0	28
BS3	LYS	CA	THR	CA	upper bound	25.0	60
BS3	GLU	CA	LYS	CA	upper bound	25.0	12
BS3	LYS	CA	MET	CA	upper bound	25.0	12
BS3	SER	CA	THR	CA	upper bound	25.0	16
BS3	ARG	CA	THR	CA	upper bound	25.0	12
BS3	ARG	CA	GLN	CA	upper bound	25.0	4
BS3	LYS	coarse-grained	TYR	coarse-grained	upper bound	25.0	24
BS3	PRO	coarse-grained	VAL	coarse-grained	upper bound	25.0	4
BS3	THR	CA	TYR	CA	upper bound	25.0	4
BS3	ALA	CA	ARG	CA	upper bound	25.0	4
BS3	TYR	CA	TYR	CA	upper bound	25.0	4
BS3	ARG	CA	MET	CA	upper bound	25.0	4
BS3	GLU	CA	THR	CA	upper bound	25.0	8
BS3	ARG	CA	LYS	CA	upper bound	25.0	20
BS3	MET	CA	TYR	CA	upper bound	25.0	8
BS3	GLN	CA	LYS	CA	upper bound	25.0	4
BS3	ALA	CA	LYS	CA	upper bound	25.0	4
BS3	GLU	CA	TYR	CA	upper bound	25.0	4
BS3	MET	CA	SER	CA	upper bound	25.0	4
BS3	ARG	coarse-grained	LYS	coarse-grained	upper bound	25.0	4

Distograms of individual restraints

Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as a minimal distance between shells; if beads intersect, the distance will be reported as 0.0. A bead with the highest available resolution for a given residue is used for the assessment.



Satisfaction of restraints

Satisfaction of restraints is calculated on a [restraint group](#) (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered satisfied, if the condition was met in at least one model of the model group/ensemble. The number of measured restraints can be smaller than the total number of restraint groups if crosslinks involve non-modeled residues. Only deposited models are used for validation right now.

State group	State	Model group	# of Deposited models/Total	Restraint group type	Satisfied (%)	Violated (%)	Count (Total=418)
1	1	1	1/28451	All	49.28	50.72	418
				Self-links/ Ambiguous	65.37	34.63	283
				Heteromeric links/ Intermolecular	15.56	84.44	135

Per-model satisfaction rates in ensembles

Every point represents one model in a model group/ensemble. Where possible, boxplots with quartile marks are also plotted.



3DEM volume

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

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